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Towards Intrinsic Molecular Communication Using Isotopic Isomerism

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Abstract

In this paper we introduce a new approach for molecular communication (MC). The proposed method uses isotopomers as symbols in a communication scenario, and we name this approach isotopic molecular communication (IMC). We propose a modulation scheme based on isotopic isomerism, where symbols are encoded via isotopes in molecules. This can be advantageous in applications where the communication has to be independent from chemical molecular concentration. Application scenarios include nano communications with isotopes in a macroscopic environment, i.e. encoding freshwater flow of rivers or drinking water utilities, or medical applications where blood carries isotopomers used for communication in a human or animal body. We simulate the capacity of communication in the sense of symbols per second and maximum symbol rate for different applications. We provide estimations for the symbol rate per distance and we demonstrate the feasibility to identify isotopes reliably. In summary, this isotopic molecular communication is a new paradigm for data transfer independent from molecular concentrations and chemical reactions, and can provide higher throughput than ordinary molecular communications.

Type of Paper and Keywords

Short communication: *molecular communication, isotopes, nanonetworks*

1 Introduction

Stable isotopes are commonly used as tracers, labels and markers besides usage of dyes and salts. They serve to investigate chemical reactions, chemical reaction pathways and biochemical metabolism clusters. Major fields of application are origin assignment of a substance and process studies aiming at improving generic aspects of a substance or of its removal and degradation [18]. With isotopes of water, the water cycle of ecosystems or watersheds can be investigated, and isotopes already have shed light on hydrological processes and strongly improved process understanding [13]. Carbon isotopes are used to investigate the carbon cycling, carbon storage and sequestration [10]. Isotope distribution measurement methods are also effective tools for food network analysis. Measurements of isotope distributions give information about sources and processes in these food webs.

In recent years research on molecular communication

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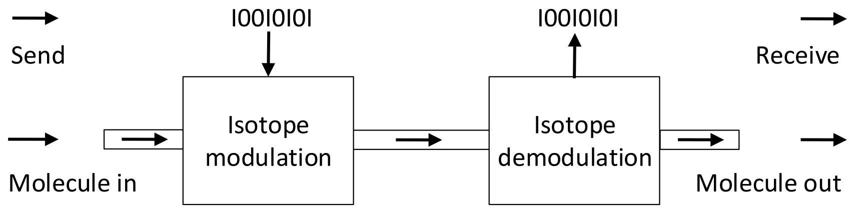

Figure 1: Principal architecture of the proposed IMC system

(MC) systems has increased in various settings from nano to macro scale [14] [6] [24] [21] [8]. Scientists working in the field of MC mainly focus on nanotechnological applications with the aim to enable communication between nanomachines [2] [1]. There are also some suggestions to apply MC in macroscale environments, as most ecological communication in ecosystems between symbiotic organisms are based on molecular communication, e.g. by plants releasing molecular stress indicators during drought [20].

In the past, accidents like the Sandoz chemical spill polluting the Rhine river have highlighted the need for intrinsic communication in resource systems as well. Parts of the water utilities along the Rhine river had to be temporarily shut down because hazardous substances contaminated the utility network and the water itself. The lack of information on when to shut down and when to re-open water facilities has demonstrated the lack of understanding travel times in such systems.

Since this incident, hydrological investigations have led to a better understanding of the water cycle in general, and of specific regional and interregional water and ecosystems. Investigations are undertaken with the aid of artificial or environmental tracers, in order to obtain information on the temporal spreading of potentially dangerous substances in the water cycle [18]. Based on these results, in the case of an accident, attempts are made to predict the arrival of substances in the drinking water network and to respond just in time with a shutdown of the utility. Still, medium- and long-term changes in the water cycle must be recorded by new hydrological measurements, which is expensive and time-consuming.

Here, a new approach is proposed, which provides an intrinsic communication system for monitoring potentially endangered water utility infrastructure.

Consequently, in this paper we propose a communication system based on molecular communication that uses isotopes and isotopomeres as symbols to increase the data rate of the resulting communication system. We name this new approach isotopic molecular communication (IMC). Its computation in principal is illustrated in Figure 1.

Encoding bits in isotopomers for data transfer increases the number of bits per symbol compared to present techniques. Isotopomers can be used for addressing, storing, controlling and authentication, or as a gateway between nano and macro communication networks.

The contributions of the paper are:

- We introduce isotopic molecular communication with encoding schemes to encode bits into isotopic symbols.
- We investigate the symbol rates for three applications via simulation of mass flow with advection and dispersion.
- We demonstrate the feasibility of the approach by introducing laser absorption spectrometry (LAS) as measuring equipment for isotropic molecular communication.

Although we still work on a complete communication system demonstrator, and the receiver is still a laboratory LAS and costly, our approach is validated by simulation and preliminary analysis, which demonstrates the feasibility of the approach. We can also observe the rapid improvement of the proposed detection system, and as it breaks down to absorption measurement with diode laser light, it is to be expected that sensor become increasingly cheaper, smaller and easier to handle.

The rest of the paper is organized as follows: Section 2 introduces related work in the field. Section 3 describes specialties of isotopic communications with an introduction to isotopes and isotopomers. We provide simulation results in Section 4 and present a suitable measuring equipment for the receiver in Section 5. We conclude the paper in Section 6 and present an outlook for future work.

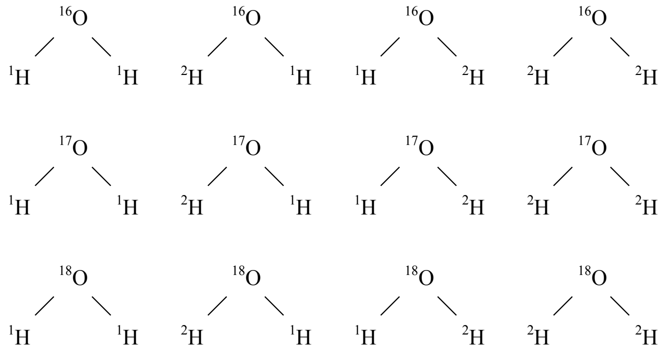

Figure 2: Water molecule as combinations of different stable ^{16}O, ^{17}O, ^{18}O, ^{1}H and ^{2}H isotopes

2 Related Work

In [7] an experimental demonstration for a digital data transmission via MC was carried out successfully. The complete MC system uses the wind speed of air for data transfer. In [12] a comparison between electromagnetic and molecular communication was presented. They figured out advantages of MC compared to electromagnetic communication and continued their work in [11], where they described a channel model for MC and developed MC physical layer techniques. [16], [17] introduced chemical molecular isomerism as a new modulation technique in MC. The authors proposed a new symbol alphabet with isomeres of glucose.

For diffusion based MC in the microscale noise channel models were worked out by [25] and [23]. And also a multiple access MC channel between multiple nano transmitters and a receiver was investigated by [22]. Tepekile et al. [26] derived an algorithm to set the threshold of a MC receiver for detection of symbols. Another approach can be to use isotopomeric isomerism in a storage device, in which data is stored in DNA strands. Storing an incredible amount of binary data > 5 Pbyte in ordinary DNA was already shown in [5].

In summary, there are many research activities in molecular communications and on detection and usage of isotopes for measurement tasks, but to the best of our knowledge we are the first to propose an (intrinsic) isotopic molecular communication system.

3 Isotopic Molecular Communication

In hydrology the abundance ratio of heavy and light isotopes of oxygen and hydrogen in relation to the observed ratios of standard mean ocean water have become a key research tool.

A number of insights into hydrological processes that could not have been obtained with other methods have been made using the stable isotopes of water. These water molecules are illustrated in Figure 2. In fact, stable isotope ratios of water carry information about age of water and the source elevation and type that persist, and can be read using laser absorption spectrometry as a detector.

A specific molecule physically consists of a specific number of elements and has a specific chemical structure. The number of elements is represented by its molecular formula, and the structure is described by its isomerism. An isotopomer is an isotopic isomer, where the position of a specific isotope in a molecule is defined. Furthermore, an isotopolog is a molecule which contains a particular number of specific isotopes. As an example we can look at the water molecule H_2O.

Theoretically water has 9 isotopologs and 12 isotopomers as shown in Figure 2, because oxygen has three stable isotopes with ^{16}O, ^{17}O and ^{18}O, and hydrogen occurs with two stable isotopes ^{1}H and ^{2}H. Practically the number of isotopomers is reduced to 9 because of the symmetry of the water molecule. Therefore, the maximum modulation order using 8 molecules is 3 bits per symbol. Of course, using liquid water for IMC is so far not possible because of the auto-dissociation of water molecules, which immediately leads to destruction of the isotopomeric information. Therefore, in liquid water only isotopologs can be used for encoding, and this maybe do not hold for nanoscale.

In general MC changes the chemical composition of a system. Isotopic communication does not necessarily do so, because information can be written intrinsically to the medium. Here, intrinsic means communication via chemicals without changing their local or distributed concentration, and this benefits to many potential

Table 1: Definition of isotopic symbols

Molecule	Symbol
$^1H_2{}^{16}O$	00
$^2H_2{}^{16}O$	01
$^1H_2{}^{18}O$	10
$^2H_2{}^{18}O$	11

applications.

Ways of using IMC could be to communicate in a free diffusive environment, in a system with forced laminar mass flow or in turbulent and chaotic systems.

3.1 Intrinsic Communication through Water Pipe

One example of an intrinsic molecular communication is a tab water transport system, which acts as medium for information transfer. On the sender side information is injected into the medium via water with different and predefined abundance ratios of ^{18}O and ^2H. Therefore, the chemical composition of the medium is not altered. On the receiver side the information is decoded via the measured abundance ratios over time, which are mapped to predefined symbols. In our case this is done by using 4 isotopologs of water, which leads to the symbol alphabet defined in Table 1.

To validate this concept we assume a simple tab water transport through a pipe with negligible diffusion and with a constant flow velocity. In this case we have to take into account dispersion and advection solely, and in which dispersion simulates also turbulent aspects. We further assume that information is injected over the whole cross-section of the pipe perpendicular to the flow direction. This system can be modelled with Equation (1), the one dimensional transport equation according to [18], which describes the concentration C of the tracer over the pipe length x and over time t:

$$D_L \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}, \tag{1}$$

where D_L is the dispersion coefficient and v is the flow velocity. To solve Equation (1) we assume an instantaneous injection at the pipe input:

$$C(x=0,t) = \frac{m}{q}\delta(t), \tag{2}$$

where m is the mass of the injected tracer and in our case the isotope labeled water, q is the volumetric flow rate and $\delta(t)$ is the Dirac function. Then the solution of Equation (1) is as follows:

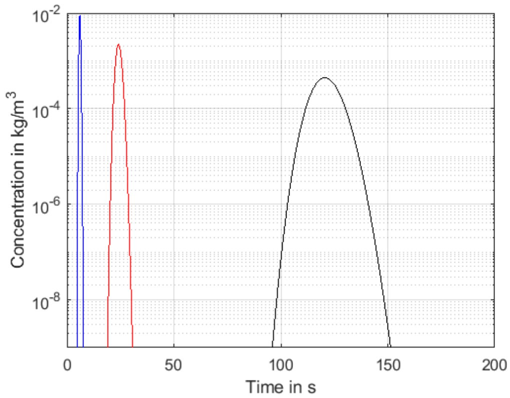

Figure 3: Concentration over time observed at the pipe lenghts $5\ m$ (blue), $20\ m$ (red) and $100\ m$ (black)

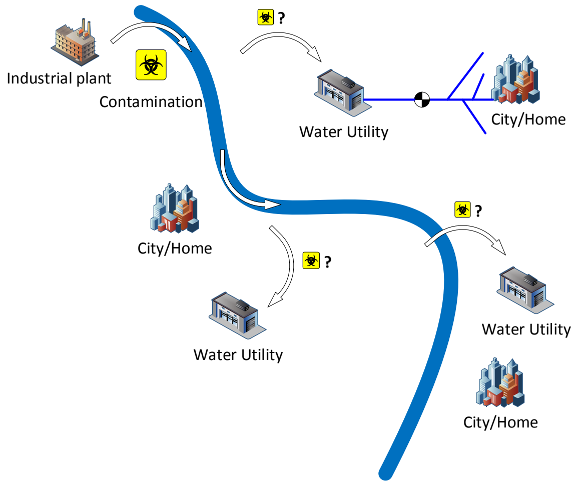

Figure 4: River contamination by pollution and endangered water utilities

$$C(x,t) = \frac{m}{q} \frac{x}{\sqrt{4\pi\ D_L\ t^3)}} exp[-\frac{(x - v\ t)^2}{4D_L\ t}] \tag{3}$$

With Equation (3) we simulated $C(x,t)$ at pipe lenghts $x_1 = 5\ m$, $x_2 = 20\ m$ and $x_3 = 100\ m$ over t. For simulation we assumed a standard tab water pipe diameter of $16\ mm$ and a standard flow rate of $q = 10\ L\ min^{-1}$. From this the velocity is calculated to $v = 0.83\ m\ s^{-1}$. D_L can be calculated with $D_L = \alpha\ v$ according to [18], whereby α is defined as longitudinal dispersivity coefficient and can be assumed to be $\alpha = 0.001 \cdot x$ in the case of a technical tab water pipe. With

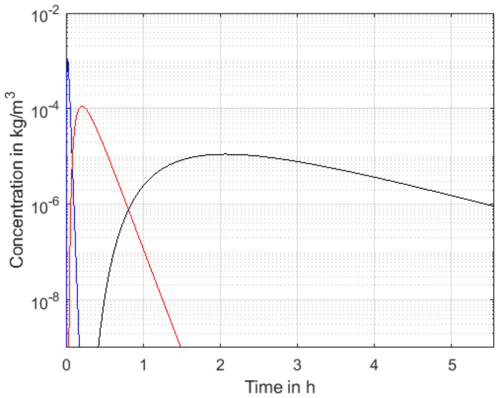

Figure 5: Simulated $C(x,t)$ distant $100\ m$ (blue), $1\ km$ (red) and $10\ km$ (black) away from the injection

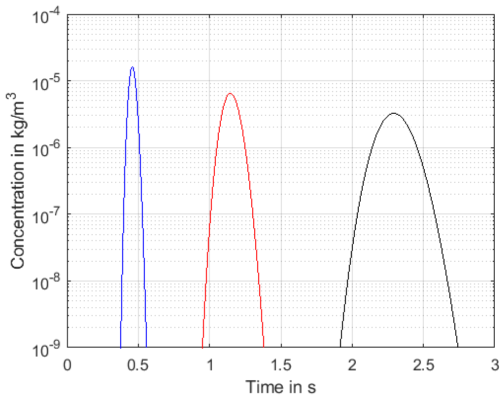

Figure 6: Brachialis artery concentration response over time at $4\ cm$ (blue), $10\ cm$ (red) and $20\ cm$ (black)

an injected tracer mass $m = 1\ g$ at $x = 0\ m$ simulation results the concentrations shown in Figure 3.

3.2 River Scenario

A possible scenario, in which an intrinsic communication system for monitoring potentially endangered water utility infrastructure is installed was already described in the introduction. The contamination of a river is illustrated in Figure 4. To simulate advection and dispersion in this scenario we applied Equation (3) once again with the same constraints as mentioned in Section 3. A typical river with a flow rate of $10\ m^3\ s^{-1}$ and a velocity of $1\ m\ s^{-1}$ was assumed, and a mass of $1\ kg$ was injected. As depicted in [18] a realistic value for the dispersivity coefficient of a typical river is $\alpha = 0.1 \cdot x$. The result of the simulation is presented in Figure 5 for river lengths $x_1 = 100\ m$, $x_2 = 1\ km$ and $x_3 = 10\ km$.

3.3 Communication in Brachialis Artery

To get an estimate of the feasible symbol rate in the human body over short distances of a few centimeters we also applied Equation (3) to the blood flow in a section of brachialis arm artery. This scenario could be useful for a communication network, for example in a network of nano machines placed at different fixed locations in the brachialis artery. Valid parameters for the simulation were taken from the literature [19], where a mean flow rate of $1.2\ mL\ s^{-1}$, a velocity of $8.7\ cm\ s^{-1}$ and a brachialis diameter of $4.3\ mm$ was measured on healthy probands at rest. We assumed the dispersivity to be $\alpha = 0.001 \cdot x$, which is thought to be a reasonable value

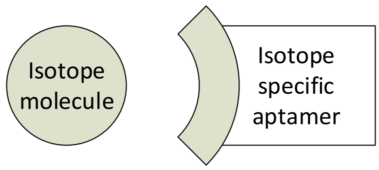

Figure 7: Hypothetical isotope detection method with an aptamer

for an artery.

With an injected mass of $1\ ng$ we obtained the simulation results shown in Figure 6. The concentration pulse widens and drops with increasing distance from the injection.

3.4 Micro Scenario

One open research question is how to detect isotopic information in a nano infrastructure to avoid large and costly devices. The key advantage of LAS is that it can operate on $< 1\ \mu L$ volumes at high measurement rates. A hypothetical isotope detection method is illustrated in Figure 7. The generation of isotopomeres in a small encoder is speculative, because easy to use single molecule synthesis is far away from practical usage. Aptamers can act as specific and selective binder for specific molecules, even at low concentrations smaller than $1\ pmol$. Hopefully aptamers can be adapted in future to isotopic sensitivity and can sorb and desorb specific isotopomeric configurations.

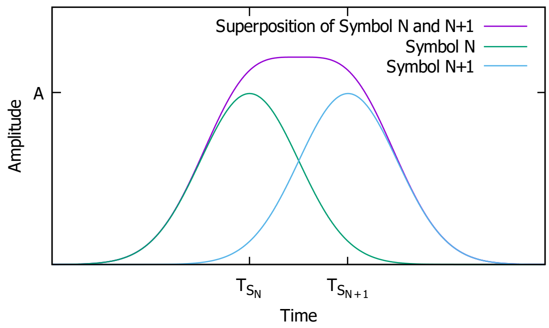

Figure 8: Intersymbol interference

4 Evaluation Results

This section provides a comparison of simulation results for the different scenarios when we build a communication system. First we will introduce the maximum symbol rate according to Nyquist theory.

To avoid intersymbol interference we suggest to create symbols so that the maximum of the symbols is 2σ apart from each other at the receiver. We allow an interference of approximately 13.5% of the symbol height according to 2σ. Consequently, the symbol duration is 2σ. This means that the symbol rate is dependent on the distance between the transmitter and the receiver as well as the channel characteristics as illustrated in Figure 3. Figure 8 illustrates the case for symbols which are perfectly gaussian shaped and the duration is exactly 2σ.

As in standard communication systems we assume that the receiver samples the symbols at the decision instants which need a synchronization between transmitter and receiver. There are applications where we do not transmit long messages as in the water utility scenario. We will handle these scenarios later in this section. With the constraint that symbols interfere if the σ becomes too large we can calculate the maximal symbol rate for different distances between transmitter and receiver.

Table 2 shows typical symbol rates and ranges of different scenarios by applying the equations to calculate the concentration and pulse shape of the signals. With the limitation of the 2 σ threshold a maximum symbol rate can be calculated.

In the use case of water utility contamination no long messages are required. Therefore, a message consist of a single symbol and symbol duration models the duration of the event, instead of sending periodic messages with the alert. For a single symbol message the receiver needs to be always on and interprets the presence of a molecule above a certain threshold concentration as an event. The advantage of our isotopic molecular communication is that although the symbol rate is very low, with many different symbols due to the usage of isotopes a number of messages can be encoded in a single symbol. According to Table 1 we define four different messages according to the bit pattern 00, 01, 10, and 11. The messages as encoded in Table 3 can be presented to the user via signal lights similar to traffic light system, so that users know how to treat the tap water. **Green** is ok and **yellow** means that the water should be boiled so that it can be used normally. **Red** means water is not drinkable.

Table 2: Symbol rate and maximum range of isotopic molecular communication in different applications

Application	Symbol Rate [Sps]		
Artery	22.2 @ 4 cm	9.3 @ 10 cm	4.7 @ 20 cm
Water pipe	2.1 @ 5 m	0.45 @ 20 m	0.09 @ 100 m
River	$9 \cdot 10^{-3}$ @ 100 m	$9 \cdot 10^{-4}$ @ 1 km	$9 \cdot 10^{-5}$ @ 10 km

Table 3: Isotopic encoding - definition of messages for tap water

Molecule	Message
${}^{1}H_2{}^{16}O$	Water without contamination (green)
${}^{2}H_2{}^{16}O$	Light bacterial contamination (yellow)
${}^{1}H_2{}^{18}O$	Strong bacterial contamination (red)
${}^{2}H_2{}^{18}O$	Chemical contamination (red)

For more complex molecules instead of water the number of bits per symbol increases as the number of isotopologs or isotopomers increases.

5 LAS Detector for IMC

The early development of stable isotope analysis was closely connected to the application of double inlet mass spectrometry to account for drift and fluctuation in measurements. Since the introduction of tunable diode laser spectrometry by [9] and [4], the technology of determining the abundance of heavy and light isotopes of hydrogen, oxygen and carbon in the molecules CO_2, H_2O has been refined and improved [3]. The key process is the detection of isotopomers using the slight difference in absorption spectra caused by vibrational and rotational movements within the molecule (asymmetric or symmetric, wagging, twisting, scissoring, and rocking).

The measurement requires diode lasers that can be fine-tuned to the precise wavelength corresponding to these energies for individual isotopomers. Fine diode

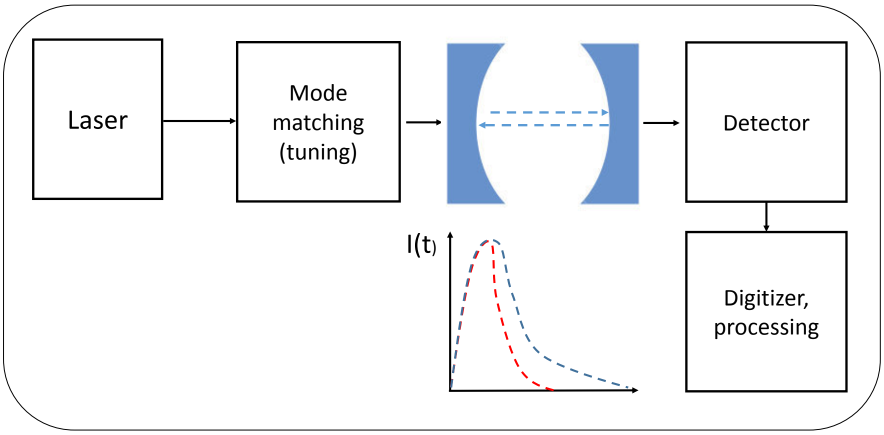

Figure 9: Laser absorption spectrometry with I(t) intensity of a vibrational or rotational mode specific wavelength

tuning is obtained by a combination of temperature and voltage modulation requiring a sophisticated temperature stabilization and voltage regulation [15]. The initial methodology of measuring the absorption of a narrow wavelength of a gas injected to a vacuum chamber between two mirrors creating a maximized optical length has been been improved by cavity ringdown spectrometry (CRS) [3]. CRS is based on the principle that the measured recession time of a specific wavelength is proportional to the abundance of that isotope. The technical principle of laser absorption spectrometry is illustrated in Figure 9.

Modern laser absorption spectroscopy can produce measurements at a sampling rate of 1 Hz. The precision of laser absorption spectrometry has reached the precision of double inlet mass spectrometry for light isotopes and for water and carbon dioxide molecules.

6 Conclusion

In this paper we have introduced isotopic molecular communication (IMC) as new concept for communication in nano- to macro-scale systems characterized by a flow of matter. The carrier substance can be air (a proven concept as for the isotopes of carbon dioxide and for vapour) or water (as for liquid water, dissolved carbon dioxide in water or dissolved gases in water). The transport of the information has been modelled using the well-established advection dispersion equation and general insights into transport length and signal density, and practical limits of the method can be obtained in future. In conclusion, the method of isotopomeric molecular communication offers significant advantages, because it introduces more combinations of symbols.

In addition, instead of using the concentration as key information, signal strength just needs to be sufficient to detect and decipher the type of isotopomer carrying the information. This increases the reach and stability of signal transmission. The discussion of three potential types of applications shows that with miniaturization and commercialization of detectors, IMC becomes a realistic option for alarm models in rivers and water distribution networks, for signal transmission in arteries and, due to the small volume required for signal detection, even in micro-fluidic applications and nanomachines. Future work will focus on prototypes and will demonstrate the encoding and decoding mechanism in air, water and real-world applications.

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